

LaOF Structure:

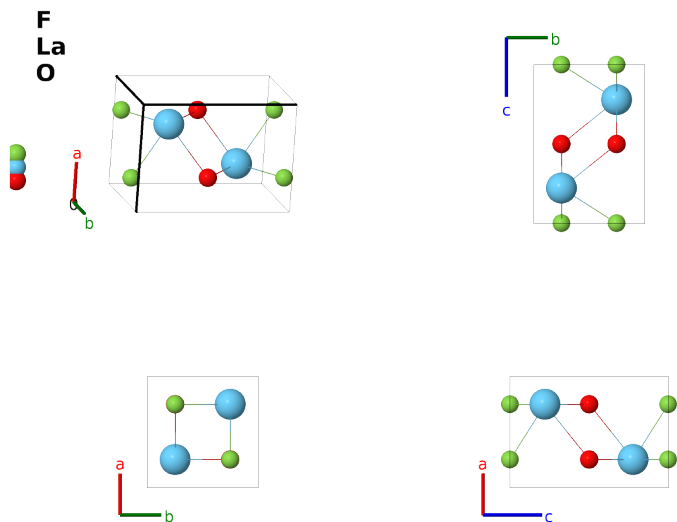
ABC_tP6_129_a_c_b-001

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<https://aflow.org/prototype-encyclopedia/JX34>

https://aflow.org/prototype-encyclopedia/ABC_tP6_129_a_c_b-001



Prototype	FLaO
AFLOW prototype label	ABC_tP6_129_a_c_b-001
ICSD	76427
CCDC	1637023
Pearson symbol	tP6
Space group number	129
Space group symbol	$P4/nmm$
AFLOW prototype command	<code>aflow --proto=ABC_tP6_129_a_c_b-001</code> <code>--params=a, c/a, z₃</code>

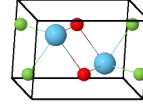
Other compounds with this structure

DyOF, ErOF, EuOF, GdOF, HoOF, LiMnAs, LiMnP, LiMnSb, NdOF, PuOF, PrOF, SmOF, TbOF, YOF

- The general formula for this compound is $\text{XO}_x\text{F}_{3-2x}$. For $x \leq 1$ the structure is tetragonal (LaOF prototype), and when $x > 1$ it is rhombohedral (YOF prototype). At high temperatures these structures transform into the cubic fluorite ($C1$) structure, with the anions statistically distributed over the $(2c)$ sites. (Zachariasen, 1951; Petzel, 1993)

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}}$	(2a)	F I
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}}$	(2a)	F I
$\mathbf{B}_3$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2c)	La I
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(2c)	La I

References

- [1] W. H. Zachariasen, *Crystal chemical studies of the 5f-series of elements. XIV. Oxyfluorides, XOF*, Acta Cryst. **4**, 231–236 (1951), doi:10.1107/S0365110X51000787.
- [2] T. Petzel, V. Marx, and B. Hormann, *Thermodynamics of the rhombohedral-cubic phase transition of ROF with R ≡ Y, La, Pr, Nd, Sm-Er*, J. Alloys Compd. **200**, 27–31 (1993), doi:10.1016/0925-8388(93)90466-Z.

Found in

- [1] J. W. Fergus, *Crystal structure of lanthanum oxyfluoride*, J. Mater. Sci. Lett. **16**, 267–269 (1997), doi:10.1023/A:1018584614532.

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